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Accelerating Newton's method

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ABSTRACT

In JCP **267**, 2014, J. Yao showed how to add a single function call to an n^{th}-order iterative algebraic solver thereby raising its order of convergence to $2n$-1. Here we generalize the scheme to arbitrarily high order, without extra derivative evaluations; and we discuss the efficiency of the schemes. For n=2 (Newton's method) and moderately large system-size M, we find a computational speed several times faster than Newton's method.

Outline

- Add a single function-evaluation to raise the order of convergence (OoC) of a root-solver from *n* to 2*n*-1.
- Efficiency and CPU time.
- Multi-step method: raise OoC to *s*(*n*-1)+1.
  - A "step" here is one new estimate of the root per iteration cycle; e.g., Newton's method is *n*=2, *s*=1.
- Results:
  - Relative efficiency cf. Newton as function of *s* and system-size *M*.
  - Example: tri-diagonal Jacobian
  - Example: Jacobian with a large condition-number
- Discussion

Add a single function-evaluation to raise the OoC from n to $2n$-1*

- Begin with an iterative algebraic solver for $f(x)=0$.
  - $f_k \equiv f(x_k)$; subscript (k) denotes iteration index.
  - For OoC n, $|x_{k+1} - x_k| = O(|x_k - x_{k-1}|^n)$.
  - Taylor series $\Longrightarrow f_k = O(|x_{k+1} - x_k|)$.
- The motivating example---raising Halley's method, n=3, to 5th order---is presented on the following page.
- The demonstration for general n is similar but with the original scheme cast in fixed-point iterative form.

*[Yao, JCP **267** (2014), 139--145]

There are two steps with this method and we demonstrate the procedure here for the case $n=3$ with the well-known Halley's method [3]. Let x_k be the kth estimate for the root. One solves the equation (assuming $f'' \neq 0$)

$$f(x_k)+f'(x_k)\delta+\frac{1}{2}f''(x_k)\delta^2=0, \tag{1}$$

and the two roots are explicitly expressed as

$$\delta=-\frac{1}{f''(x_k)}\left(f'(x_k)\pm\sqrt{f'(x_k)^2-2f(x_k)f''(x_k)}\right).$$

To recover Newton's method [2] when the quadratic term vanishes, we pick only one root and it can be written as

$$\delta=\frac{\operatorname{sgn}(f'(x_k))}{f''(x_k)}\left(\sqrt{\left(f'(x_k)\right)^2-2f(x_k)f''(x_k)}-\left|f'(x_k)\right|\right).$$

The above step uses three functional calls. Note that a Taylor series for $f(x+\delta)$ at $x=x_k$ using Eq. (1) implies

$$f(x_k+\delta)=O\left(\delta^3\right). \tag{2}$$

The next step uses one more function call to gain two more orders of convergence. One adds a term $f(x_k+\delta)$ to Eq. (1), and solves

$$f(x_k+\delta)+f(x_k)+f'(x_k)\Delta+\frac{1}{2}f''(x_k)\Delta^2=0. \tag{3}$$

The solution is similar to that obtained in the first step:

$$\Delta=\frac{\operatorname{sgn}(f'(x_k))}{f''(x_k)}\left(\sqrt{\left(f'(x_k)\right)^2-2\left(f(x_k+\delta)+f(x_k)\right)f''(x_k)}-\left|f'(x_k)\right|\right).$$

Finally, let $x_{k+1}=x_k+\Delta$ for completion of the current iteration cycle.

One computes only four function values $f(x_k)$, $f'(x_k)$, $f''(x_k)$, and $f(x_k+\delta)$. However, the above scheme is fifth order convergent as shown next.

From a Taylor expansion one obtains

$$f(x_k+\Delta)=f(x_k)+f'(x_k)\Delta+\frac{1}{2}f''(x_k)\Delta^2+\frac{1}{6}f'''(x_k)\Delta^3+O\left(\Delta^4\right).$$

The sum of the first three terms in the right-hand side is equal to $-f(x_k+\delta)$ from Eq. (3); thus $f(x_k+\Delta)=-f(x_k+\delta)+f'''(x_k)\Delta^3/6+O(\Delta^4)$. However, from Eq. (1) and the Taylor expansion of $f(x_k+\delta)$, the above estimate becomes

$$f(x_k+\Delta)=\frac{1}{6}f'''(x_k)\left(\Delta^3-\delta^3\right)+O\left(\Delta^4-\delta^4\right)=(\Delta-\delta)O\left(\Delta^2,\delta^2\right). \tag{4}$$

By subtracting Eq. (1) from Eq. (3) one arrives at

$$(\Delta-\delta)\left(f'(x_k)+O(\delta)\right)=-f(x_k+\delta)=O\left(\delta^3\right). \tag{5}$$

It tells us that Δ and δ are of the same order and

$$(\Delta-\delta)=O\left(\delta^3\right).$$

One easily sees from Eq. (4) and Eq. (5) that

$$f(x_{k+1})=f(x_k+\Delta)=O\left(\Delta^5\right).$$

Therefore the method is *fifth-order* convergent; however it employs only *four* function values. The proof above can be generalized for arbitrary n.

Efficiency of function-evaluations and CPU cost

- Higher-order methods require more *f*-evaluations $\Longrightarrow$ often *not* more computationally efficient:
  - Two iterations reduce the error by $(f_k{}^n)^n \sim f_k{}^{(n\wedge 2)}$, not $\sim f_k{}^{2n}$.
    - n^n: fairly rapid error-reduction even at low n.
    - If f is expensive it can be cheaper to take more iterations than to accomplish more per more costly iteration.
- $\mathcal{E}_f$, the error-reduction per function-evaluation, was introduced by early authors to analyze efficiency.

Efficiency and CPU cost, cont.

- $\mathcal{E} \equiv$ error-reduction exponent after k iterations: $\mathcal{E} = n^k$.
- $N_T \equiv$ total no. of f-evaluations to reach a given $\mathcal{E}$:
  $N_T = kN_1$, where N_1 is no. of f-evaluations per iteration.
- Then $\mathcal{E} = n^{N\_T/N\_1} = (n^{1/N\_1})^{N\_T}$, so that $\mathcal{E}_f = n^{1/N\_1}$.
  - $M = 1$ examples (assume cost of f', etc. ~ f):
    - Any 1-step method: Taylor series for $f \Longrightarrow \mathcal{E}_f = n^{1/n}$.
    - Page 4: $\mathcal{E}_f = (2n\text{-}1)^{1/(n+1)}$.
- C_{CPU}, $C_{\text{CPU}f} \equiv$ computational cost to realize $\mathcal{E}$, evaluate f:
  - $C_{\text{CPU}} = N_T C_{\text{CPU}f} = C_{\text{CPU}f} \ln \mathcal{E} / \ln \mathcal{E}_f \longrightarrow_{(\mathcal{E}\_f \sim 1)} C_{\text{CPU}f} \ln \mathcal{E} / (\mathcal{E}_f - 1)$.

Multi-step method: raise OoC to *s*(*n*-1)+1

III. GENERALIZATION OF THE ACCELERATION SCHEME TO FIXED-POINT ITERATIVE METHODS

Acceleration of $n > 2$ Taylor-series-based root-solvers, while achieving convergence of order $2n-1$ with $n+1$ function-evaluations, has the drawback in common with the original solver that roots of polynomials of degree $n-1$ must be solved for the intermediate and final step-sizes; and the appropriate roots from these solves must be identified. Here we circumvent these complications by developing the acceleration method for fixed-point iteration: One solves for $f(x)=0$ by iterating upon x_k according to

$$x_{k+1} \;=\; x_k + \delta_k \tag{2}$$

with $\delta_k = \delta(f_k, f'_k, f''_k, \ldots)$, where $f_k \equiv f(x_k)$, $f'_k \equiv f'(x_k)$, $f''_k \equiv f''(x_k)$, etc. Without loss of generality, δ can be written in the form

$$\delta \;=\; -\frac{f}{f'}(1+g)\,, \tag{3}$$

with $g = g(f, f', f'', \ldots)$ and $g_k \equiv g(f_k, f'_k, f''_k, \ldots)$. The iteration scheme is said to be n^{th}-order convergent if

$$f_{k+1} \;\sim\; \mathcal{O}(\delta_k^n)\,. \tag{4}$$

The Taylor expansion of f_{k+1} then becomes (employing the alternate notation $f^{(i)}$ for the i^{th} derivative of f where convenient):

$$f_{k+1} = \sum_{i=0}^{\infty} f_k^{(i)} \frac{\delta_k^i}{i!} = -f_k g_k + \sum_{i=2}^{\infty} \frac{f_k^{(i)}}{i!}\left(\frac{-f_k}{f'_k}\right)^i (1+g_k)^i\,. \tag{5}$$

In the second equality, note that $f_k g_k$, the remainder of the two lowest-order terms, can be at most of second order (since $f_{k+1} \sim \mathcal{O}(\delta_k^n)$), which then implies $f_k \sim \delta_k$, which in turn restricts g_k to at most first order. The series is in the form of a function, h, that is analyzed in the Appendix. It is shown there what conditions g must satisfy in order that $f_{k+1} \sim \mathcal{O}(\delta_k^n)$.

We now apply our acceleration approach to this fixed-point iteration. The functions f, g, and δ will remain the same. To distinguish the modified iterates, we will use use tilde's, i.e., $\tilde\delta_k \equiv \delta(\tilde f_k, \tilde f_k{}', \tilde f_k{}'' \ldots)$, $\tilde f_k \equiv f(\tilde x_k)$, $\tilde f_k{}' \equiv f'(\tilde x_k)$, $\tilde g_k \equiv g(\tilde f_k, \tilde f_k{}', \tilde f_k{}'' \ldots)$, etc. We set

$$\tilde x_{k+1} = \tilde x_k + \Delta_k$$

with

$$\Delta_k = -\frac{\tilde f_k + f^*}{\tilde f_k{}'}(1+g^*)$$
$$g^* \equiv g(\tilde f_k + f^*, \tilde f_k{}', \tilde f_k{}'' \ldots)$$

and

$$f^* \equiv f(\tilde x_k + \tilde\delta_k) = \sum_{i=0}^{\infty} \tilde f_k{}^{(i)} \frac{\tilde\delta_k^i}{i!} = -\tilde f_k \tilde g_k + \sum_{i=2}^{\infty} \frac{\tilde f_k{}^{(i)}}{i!}\left(\frac{-\tilde f_k}{\tilde f_k{}'}\right)^i (1+\tilde g_k)^i\,.$$

We then have

$$\tilde{f}_{k+1} = \sum_{i=0}^{\infty} \tilde{f}_k^{\,(i)} \frac{\Delta_k^i}{i!} = -f^* - (\tilde{f}_k + f^*)\, g^* + \sum_{i=2}^{\infty} \frac{\tilde{f}_k^{\,(i)}}{i!} \left(\frac{-(\tilde{f}_k + f^*)}{\tilde{f}_k^{\,\prime}} \right)^i (1+g^*)^i \,. \tag{6}$$

In the second equality, observe that both f^* and the remaining terms are each in the form of the function h introduced as the right-hand-side of Eq. (5). Thus the results of the Appendix can be applied to them. This gives their scalings as order $\tilde{f}_k^{\,n}$ and $(\tilde{f}_k + f^*)^n \sim \tilde{f}_k^{\,n}$ respectively, and Eq. (A7) is then used to obtain

$$\tilde{f}_{k+1} = \mathcal{O}(f^* \times \max(f^*, \tilde{f}_k)^{n-1}) = \mathcal{O}(\tilde{f}_k^{\,2n-1}).$$

As in Ref. [1], with a cost of a single additional function-evaluation, the convergence of the original n^{th}-order method has been raised to $2n-1$.

To complete contact with Ref. [1], we also calculate

$$(\Delta_k - \tilde{\delta}_k)\tilde{f}_k^{\,\prime} = (\tilde{g}_k - g^*)\tilde{f}_k - (1+\tilde{g}_k) f^* \sim -\tilde{f}_k \tilde{g}^{(1)} f^* - f^* \sim f^* \sim \mathcal{O}(\tilde{\delta}_k^n).$$

IV. INCREASING THE CONVERGENCE-RATE FURTHER WITHOUT ADDITIONAL DERIVATIVE EVALUATIONS

In this section we consider additional function evaluations (but no additional derivative evaluations) in going from f_k to f_{k+1} with a fixed-point iterative method. Our primary interest is to accelerate schemes for large systems (which typically call for $n=2$ to avoid the expense of derivatives beyond the first), but we begin with general n and with a scalar f for simplicity (the generalization to $M>1$ is straightforward).

We begin with some new notation. The subscript k will be dropped; all quantities should be understood to be at iteration k unless explicitly noted otherwise. Similarly the tilde ($\tilde{}$), denoting a modified method's iterates (as opposed to the original's, i.e., with Taylor series (5)) will be dropped. We identify step quantities with a bar ($\bar{}$) and the step index with a capitalized Roman-numeral superscript; and we define s to be the number of steps. We map our new variables onto the accelerated fixed-point method of Sec. III:

$$\begin{aligned}
\bar{x}^{\mathrm{S_0}} &\leftrightarrow \tilde{x}_k \\
\bar{f}^{\mathrm{S_0}} &\leftrightarrow \tilde{f}_k \\
\bar{A}^{\mathrm{S_0}} &\leftrightarrow \tilde{f}_k \\
\bar{g}^{\mathrm{S_0}} &\leftrightarrow \tilde{g}_k = g(\tilde{f}_k, \tilde{f}_k^{\,\prime}, \tilde{f}_k^{\,\prime\prime} \ldots) \\
\bar{\delta}^{\mathrm{S_0}} &\leftrightarrow \tilde{\delta}_k = -(\tilde{f}_k/\tilde{f}_k^{\,\prime}) \times (1+\tilde{g}_k) \\
\\
\bar{x}^{\mathrm{S_I}} &\leftrightarrow x^* = \tilde{x}_k + \tilde{\delta}_k \\
\bar{f}^{\mathrm{S_I}} &\leftrightarrow f^* = f(x^*) \\
\bar{A}^{\mathrm{S_I}} &\leftrightarrow \tilde{f}_k + f^* \\
\bar{g}^{\mathrm{S_I}} &\leftrightarrow g^* = g(\tilde{f}_k + f^*, \tilde{f}_k^{\,\prime}, \tilde{f}_k^{\,\prime\prime} \ldots) \\
\bar{\delta}^{\mathrm{S_I}} &\leftrightarrow \Delta_k = -((\tilde{f}_k + f^*)/\tilde{f}_k^{\,\prime}) \times (1+g^*) \\
\\
\bar{x}^{\mathrm{S_{II}}} &\leftrightarrow \tilde{x}_{k+1} = \tilde{x}_k + \Delta_k \\
\bar{f}^{\mathrm{S_{II}}} &\leftrightarrow \tilde{f}_{k+1} = f(\tilde{x}_{k+1}),
\end{aligned}$$

where we have introduced the new variable $\bar{A}^{\mathrm{S_i}} \equiv \sum_{j=0}^{i} \bar{f}^{\mathrm{S_j}}$.

We write the new scheme (omitting updates of quantities which simply follow their definitions, such as $\bar{f}^{\mathrm{S_{i+1}}} =$

$f(\bar{x}^{\mathrm{S}_{\mathrm{i+1}}})$):

$$\begin{aligned}
\bar{x}^{\mathrm{S}_0} &= \bar{x} \\
\bar{g}^{\mathrm{S}_0} &= g(\bar{A}^{\mathrm{S}_0}, f', f'', \dots) \\
\bar{\delta}^{\mathrm{S}_0} &= -(\bar{A}^{\mathrm{S}_0}/f') \times (1 + \bar{g}^{\mathrm{S}_0}) \\
\\
\bar{x}^{\mathrm{S}_\mathrm{i}} &= \bar{x} + \bar{\delta}^{\mathrm{S}_{\mathrm{i\text{-}1}}} \\
\bar{g}^{\mathrm{S}_\mathrm{i}} &= g(\bar{A}^{\mathrm{S}_\mathrm{i}}, f', f'', \dots) \\
\bar{\delta}^{\mathrm{S}_\mathrm{i}} &= -(\bar{A}^{\mathrm{S}_\mathrm{i}}/f') \times (1 + \bar{g}^{\mathrm{S}_\mathrm{i}}) \\
\\
\bar{x}^{\mathrm{S}_s} &= \bar{x} + \bar{\delta}^{\mathrm{S}_{s\text{-}1}} \\
x_{k+1} &= \bar{x}^{\mathrm{S}_s},
\end{aligned} \tag{7}$$

giving for the Taylor expansion of f_{k+1}:

$$f_{k+1} = \sum_{i=0}^{\infty} f^{(i)} \frac{(\bar{\delta}^{\mathrm{S}_{s\text{-}1}})^i}{i!} = f - (1 + \bar{g}^{\mathrm{S}_{s\text{-}1}})\bar{A}^{\mathrm{S}_{s\text{-}1}} + \sum_{i=2}^{\infty} \frac{f^{(i)}}{i!} \left(\frac{-\bar{A}^{\mathrm{S}_{s\text{-}1}}}{f'} \right)^i \left(1 + \bar{g}^{\mathrm{S}_{s\text{-}1}}\right)^i = f - \bar{A}^{\mathrm{S}_{s\text{-}1}} + \bar{h}^{\mathrm{S}_{s\text{-}1}}. \tag{8}$$

To proceed, we develop an iterative relation for the steps from the intermediate Taylor series, beginning with:

$$\bar{f}^{\mathrm{S}_{\mathrm{i+1}}} = f - \bar{A}^{\mathrm{S}_\mathrm{i}} + \bar{h}^{\mathrm{S}_\mathrm{i}}.$$

Subtracting the series for $\bar{f}^{\mathrm{S}_\mathrm{i}}$ gives:

$$\bar{f}^{\mathrm{S}_{\mathrm{i+1}}} - \bar{f}^{\mathrm{S}_\mathrm{i}} = -\bar{A}^{\mathrm{S}_\mathrm{i}} + \bar{A}^{\mathrm{S}_{\mathrm{i\text{-}1}}} + \bar{h}^{\mathrm{S}_\mathrm{i}} - \bar{h}^{\mathrm{S}_{\mathrm{i\text{-}1}}},$$

so that

$$\bar{f}^{\mathrm{S}_{\mathrm{i+1}}} = \bar{h}^{\mathrm{S}_\mathrm{i}} - \bar{h}^{\mathrm{S}_{\mathrm{i\text{-}1}}} \sim (\bar{A}^{\mathrm{S}_\mathrm{i}} - \bar{A}^{\mathrm{S}_{\mathrm{i\text{-}1}}})\, \mathcal{O}(f^{n-1}) \sim \bar{f}^{\mathrm{S}_\mathrm{i}}\, \mathcal{O}(f^{n-1}) \sim \mathcal{O}(f^{(i+1)(n-1)+1}),$$

where we have used Eq. (A7). Using this result in Eq. (8), we obtain the convergence rate:

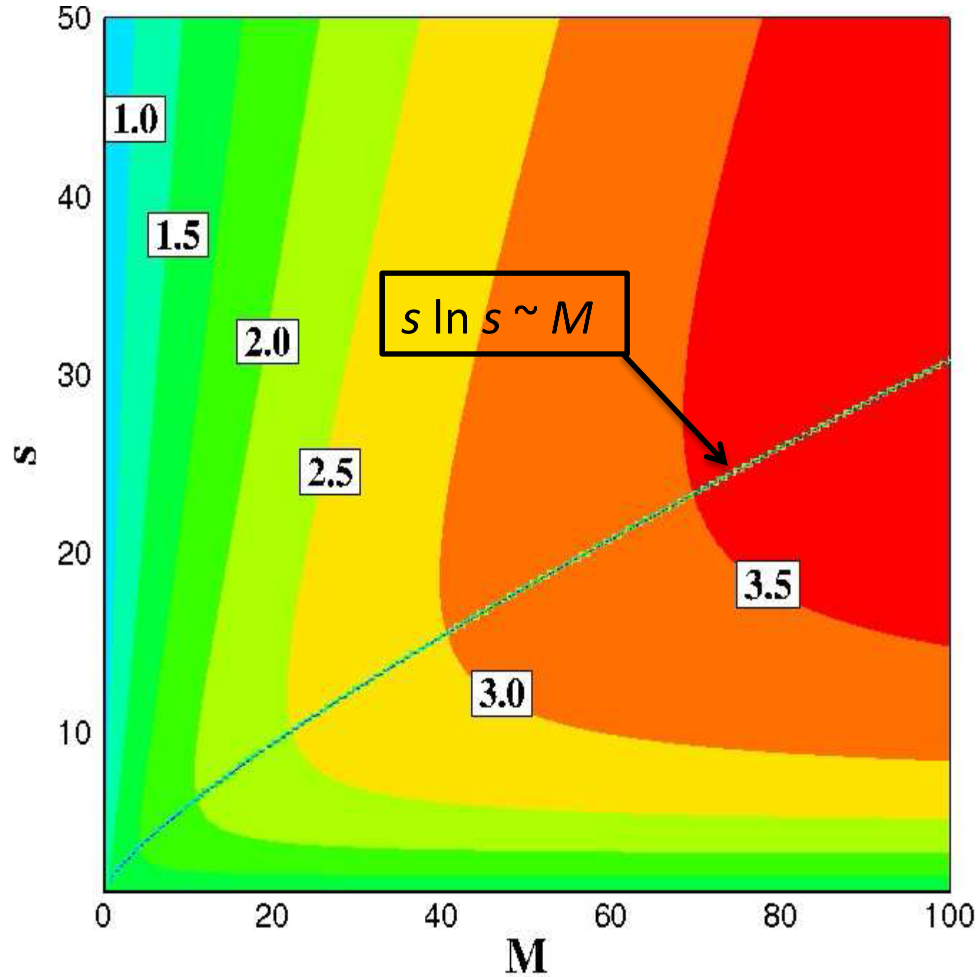
$$f_{k+1} \sim \mathcal{O}(f^{s(n-1)+1}), \tag{9}$$

having evaluated one derivative and s f-functions.

The error-reduction per function-evaluation of this scheme, assuming f' costs about the same as f to evaluate, is $\mathcal{E}_f = (s(n-1)+1)^{1/(n+s-1)}$. Evaluations of $\mathcal{E}_f$ at small s and n reveal a single maximum, $\mathcal{E}_f = 1.495$ at $s = 2$, $n = 3$, i.e., at the first case analyzed in [1]—Halley's scheme accelerated to 5$^{\mathrm{th}}$-order. For comparison, the original Halley's scheme, $s = 1$, $n = 3$, has $\mathcal{E}_f = 1.442$.

Accelerated Newton scheme shows continuous improvement with *s*

- Plotted are contours of constant $(\mathcal{E}_f(s,M)-1)/(\mathcal{E}_f(1,M)-1)$: the relative efficiency of the *s*-step scheme cf. Newton
  - Improvement over Newton is above a factor of 3 for *M* above 40.
  - $d\mathcal{E}_f/ds = 0 \Rightarrow s \ln s \sim M$: a good fit to the optimum *s* at given system-size.
  - Improvement continues as $M \longrightarrow \infty$.



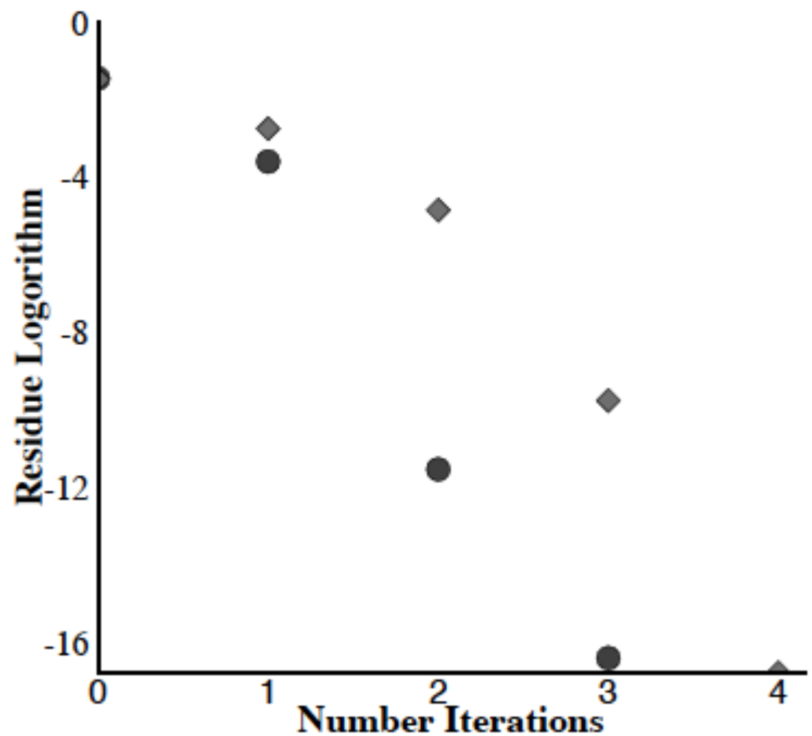
Example: tri-diagonal system

$$
\begin{aligned}
x_1 + \frac{1}{2}\sin(x_2) &= 1.0; \\
\frac{1}{2}\sin(x_1) \;+\; x_2 \;+\; \frac{1}{2}\sin(x_3) &= 1.0; \\
\ldots \quad \ldots &= \ldots \\
\frac{1}{2}\sin(x_{i-1}) \;+\; x_i \;+\; \frac{1}{2}\sin(x_{i+1}) &= 1.0; \\
\ldots \quad \ldots &= \ldots \\
\frac{1}{2}\sin(x_{M\text{-}1}) \;+\; x_M &= 1.0.
\end{aligned}
$$

- We solve this system with n=2, s=3 and M=32.
  - 8-byte arithmetic
  - Jacobian is inverted by back-substitution

tri-diagonal system, cont.

- Initial guess: x_i=1/2
- Residuals follow predicted convergence rates---parabola (diamonds) and cubic (circles) for Newton and accelerated Newton respectively.
  - Final iterations have reached machine accuracy.



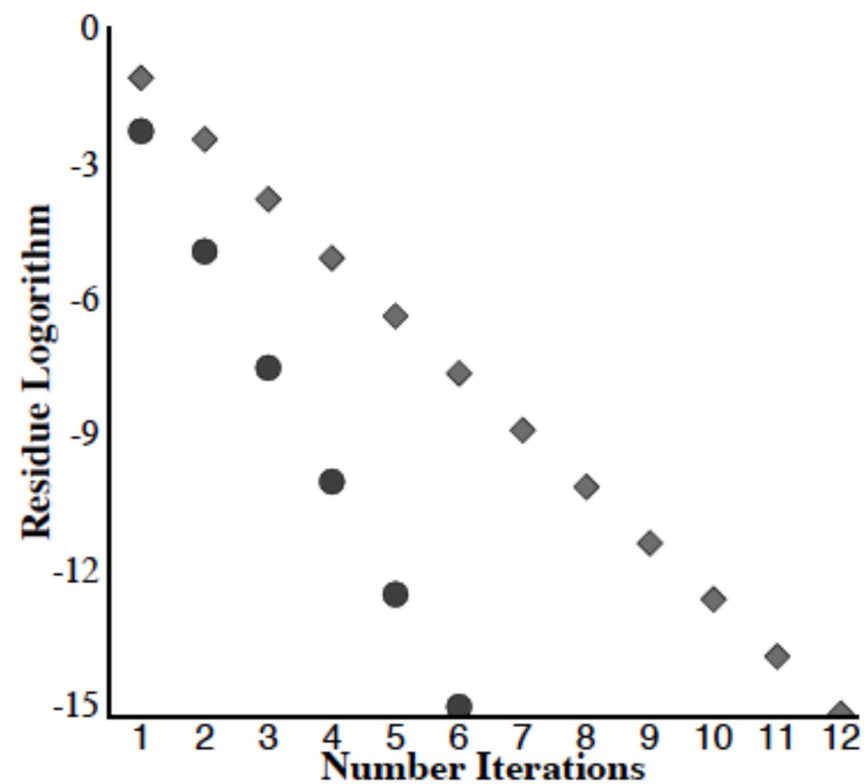
Example: ill-conditioned Jacobian

$$Mx_i + \sum_{j=1}^{M} \frac{\sin(x_i + x_j)}{i + j - 1} = \frac{M}{i} + \sum_{j=1}^{M} \frac{\sin(\frac{1}{i} + \frac{1}{j})}{i + j - 1}$$

- Solution is $x_i = 1/i$.
- We solve with n=2, s=3 and M=32.
  - 8-byte arithmetic
  - We use Cholesky decomposition of the Jacobian. Large condition-number ⇒ inverse is inaccurate

ill-conditioned Jacobian, cont.

- Initial guess: $x_i = x_{si} * (1+.5\ r_i)$
  - r_i = random number in [-1,1]
- Both the Newton and accelerated Newton schemes achieve only linear convergence due to finite accuracy of the Jacobian matrix decomposition.
- Accelerated scheme nevertheless still provides a significant advantage.



Summary/Discussion

- We have extended [Yao, JCP 2014 (s=2)] to an arbitrary number of steps s per iteration and estimated the error-reduction per function-evaluation, $\mathcal{E}_f$, and computational cost, C_{CPU}, of the methods.
  - No extra derivative-evaluations are needed.
  - The OoC is accelerated from the original order n to order $s(n\text{-}1)+1$.
  - M = 1: $\mathcal{E}_f = (s(n-1)+1)^{1/(n+s-1)}$.
    - At small n, $\mathcal{E}_f$ has a single maximum – at small s. For n=3, s_{max}=2 (which turns out to be the page 5 case). $\mathcal{E}_f$ goes from = 1.442 to 1.495 : small improvement.
  - $M > 1$, n=2: $\mathcal{E}_f = (s+1)^{1/(M(s+M))}$:
    - For $s \ll M$, $\mathcal{E}_f$ increases with s. Optimum s occurs at $s \ln s \sim M$: Leads to significant improvement in C_{CPU} for large M.
- Even when the Jacobian of an originally 2nd-order method is ill-conditioned and the theoretical OoC is not achieved, the new scheme can reduce the original C_{CPU} by a factor of two.